Silicon Carbide Epitaxial Layer Thickness Measurement Based on Infrared Interferometry Method and Simulated Annealing-Least Squares Hybrid Optimization Algorithm

Pengyu Zhu[1,a,#], Zidong Yi[2,b,#]

[1]School of Energy and Power Engineering, Xi'an Jiaotong University, Xi'an, Shaanxi, China

[2]School of Software, Xi'an Jiaotong University, Xi'an, Shaanxi, China

[a]3367768286@qq.com, [b]jfm200408@stu.xjtu.edu.cn

[#]These authors contributed equally to this work.

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Abstract: As a third-generation semiconductor material, silicon carbide (SiC) epitaxial layer thickness is a key parameter to measure material quality and device performance. In order to achieve accurate and non-destructive measurement of its thickness, a systematic measurement and optimization model was constructed based on infrared interferometry. In the first step, a simplified dual-beam interferometric physical model is established. The model considers the single reflection and transmission of light waves at the interface between the epitaxial layer and the substrate, and inverts the thickness of the epitaxial layer by analyzing the interference fringes in the reflection spectrum. In order to accurately describe the optical properties of materials, the Sellmeier equation and the Drude model are introduced to describe the dispersion effect of silicon carbide refractive index with wavelength and carrier concentration, and the theoretical calculation formula of epitaxial layer thickness is derived by combining Snell's law and interference conditions. In the second step, based on the model of the first step, a thickness calculation and optimization algorithm combining least squares method and simulated annealing algorithm is designed. The algorithm optimizes the thickness value by minimizing the error function between the theoretical and measured reflectances, and the simulated annealing algorithm is used to avoid the local optimal solution to ensure the global nature of the solution. In order to deal with the randomness of s-polarized and P-polarized light in actual measurements, the average reflection coefficient of the two is used in the calculation. The algorithm was applied to process the experimental data, and the calculated average thickness of the bright pattern was 9.93 μm and 9.79 μm, the average thickness of the dark pattern was 11.29 μm and 10.91 μm, and the thickness difference was 12.75% and 10.84%, respectively, when the incidence angle was 10° and 15°, the results were in good agreement, which verified the effectiveness and accuracy of the model.

1. Introduction

Silicon carbide (SiC) has shown great application potential in the field of high-temperature, high-frequency, and high-power electronic devices due to its excellent physical and chemical properties such as wide bandgap, high critical breakdown electric field, and high thermal conductivity, and has become a representative of the third generation of semiconductor materials [1]. In the preparation of epitaxial materials and device fabrication, the thickness of the epitaxial layer is one of the core parameters that directly affects the electrical performance, reliability and yield of the device. Therefore, the development of an accurate, efficient, and non-destructive thickness measurement technology is crucial for optimizing the epitaxial growth process of materials and improving the performance of the final device.

Among many non-destructive testing techniques, infrared interferometry is widely used due to its advantages such as easy operation, high efficiency and no damage to the sample [2]. The basic

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principle is that when infrared light shines on the epitaxial sheet, reflection and transmission will occur at the interface between the epitaxial layer and the substrate. Due to the difference in refractive index between the epitaxial layer and the substrate, there is a path difference between the beams reflected at different interfaces, and when these beams meet, interference effects will occur, forming periodic interference fringes in the reflection spectrum. The period, phase and amplitude information of these interference fringes are closely related to the thickness and refractive index of the epitaxial layer. By analyzing the interference spectrum, combined with the known information such as the angle of incident light and the refractive index of the material, the thickness of the epitaxial layer can be calculated by inversion. However, in practical applications, the refractive index of epitaxial layer materials is not constant, and it will have a significant dispersion effect with the change of incident light wavelength and the concentration of carriers within the material, which poses challenges to the accuracy of traditional measurement models [3].

In order to solve the above problems and achieve accurate measurement of silicon carbide epitaxial layer thickness, this research work is divided into two core steps. The first step is to establish an accurate interferometric physical model. We start with the simplified two-beam interference hypothesis, that is, only consider the interference generated by the primary reflection of light at the upper and lower interfaces of the epitaxial layer. Under this framework, the phase conditions of interference fringes (light and dark lines) are deeply analyzed, and the mathematical relationship between thickness and interference series, wavelength and refractive angle is derived. Crucially, the model successfully describes the complex relationship between silicon carbide refractive index with wavelength and carrier concentration by introducing the Sellmeier equation [4] and the Drude model [5], providing a more realistic physical basis for thickness inversion. The second step focuses on transforming physical models into actionable, robust computational algorithms. Based on the mathematical model established in the first step, we design a complete set of thickness calculation algorithm flow. The core of the algorithm is to use optimization theory to minimize the difference between the theoretical calculated reflectance and the experimentally measured reflectance. We use the least squares method to construct the objective function, and innovatively introduce the simulated annealing algorithm for global optimization solving [6], which effectively avoids the problem of falling into local optimum due to the nonlinearity of the objective function. Through the processing and analysis of experimental data, the algorithm can stably output the thickness estimate of the epitaxial layer, and verify the consistency and reliability of the proposed method by comparing the results at different angles of incidence [7].

2. Model creation, solution and discussion

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2.1. Model establishment

2.1.1. Dual-beam interference physics model

Based on the principle of infrared interference, a two-beam interference model for measuring the thickness of silicon carbide epitaxial layer was established. When infrared light is incident on the epitaxial layer surface at an angle θ, the interference of two beams of reflected light is mainly considered: one beam is reflected directly from the air-epitaxial layer interface (light 1), and the other beam first transmits into the epitaxial layer, reflects at the epitaxial layer-substrate interface, and then transmits back into the air (light 2). The two beams of light have different paths due to different propagation paths, resulting in interference fringes.

The relationship between the optical path difference Δ and the interference extreme point is (considering half-wave loss):

$$2n(\lambda,C)L\ cos\ \theta t\ =\ (m\ -\ 1/2)\lambda \tag{1}$$

where L is the thickness of the epitaxial layer to be found, n(λ,C) is the refractive index of the epitaxial layer that depends on the wavelength λ and the carrier concentration C, θt is the angle of refraction, and m is the interference series.

An accurate description of the refractive index n(λ,C) is key to the model. In this study, the Sellmeier equation and the Drude model were used combined:

The Sellmeier equation describes the intrinsic dispersion:

$$n_2(\lambda)\ =\ 1\ +\ B_1\lambda_2/(\lambda_2\ -\ C_1) \tag{2}$$

where B1 ≈ 5.5394 and C1 ≈ 0.026945 μm² are the dispersion constants of silicon carbide.

The Drude model describes the effects of carrier concentration:

$$n(\lambda,C)\ =\sqrt{[\varepsilon_\infty-\ (C\ e^2)/(2\pi\varepsilon_0\ m^*\lambda^2)]} \tag{3}$$

where $\varepsilon_\infty\ =\ 6.52$ is the high-frequency dielectric constant, e is the electron charge, ε_0 is the vacuum dielectric constant, and m is the electron effective mass.

According to Snell's law $n_0\ sin\ \theta\ =\ n(\lambda,C)\ sin\ \theta t$ (where n_0= 1 is the refractive index of air), the solution equation of the interference series m can be established, and then the expression of thickness L can be derived:

$$L\ =\ m_0\lambda_m/\ [2n(\lambda_m,C)\sqrt{(1\ -\ (sin\theta/n(\lambda_m,C))^2)}] \tag{4}$$

To reduce the random error, the average value of the thickness calculated for multiple adjacent extreme points is $L_{avg}\ =\ \frac{1}{M}\sum_i^M L_i$.

2.1.2. Design of optimized algorithm for thickness calculation

Based on the above physical model, an optimization algorithm for inverting thickness is designed. The core idea of the algorithm is to find a thickness L so that the overall error between the theoretical reflectance R_{calc} calculated based on this thickness and the experimentally measured reflectance R_{meas} is minimal.

First, the theoretical reflectance needs to be calculated. For s-polarized and P-polarized light, the reflection coefficients R_s and R_p are given by the Fresnel formula:

$$R_s\ =\ [(n_1\ cos\ \theta_1\ -\ n_2\ cos\ \theta_2)/(n_1\ cos\ \theta_1\ +\ n_2\ cos\ \theta_2)]^2 \tag{5}$$

$$R_p\ =\ [(n_2\ cos\ \theta_2\ -\ n_1\ cos\ \theta_1)/(n_2\ cos\ \theta_2\ +\ n_1\ cos\ \theta_1)]^2 \tag{6}$$

Considering the uncertainty of the polarized state of the incident light, the average of the two is taken as the total reflectance: $R_{total}\ =\ (R_s\ +\ R_p)/2$.

The objective function is constructed as the sum of the squares of the weighted residuals:

$$f(L)\ =\sum_1^K w_k\ [R_{calc}(\lambda_k;\ L)\ -\ R_{meas}(\lambda_k)]^2 \tag{7}$$

w_k is the weight coefficient, which can be appropriately reduced in high-noise areas to improve the stability of the algorithm.

In order to solve the optimization problem, the two-scale computation-data inversion algorithm is used:

Global search (macro scale): Simulated annealing algorithm is used to conduct a global search within the thickness prior interval $\left[L_{min},\ L_{max}\right]$. Simulated annealing accepts the new solution with the probability $P\ =\ min\left\{1,\ \exp\left(\left[f\left(L\right)\ -f\left(L'\right)\right]/T_t\right)\right\}$ through the Metropolis criterion, so that it has the ability to jump out of the local minimum point and find the regional L_{macro} where the global optimal solution is located.

Local optimization (microscale): Using L_{macro} as the initial value, an efficient nonlinear least squares algorithm is used for fine optimization to obtain the final optimal thickness estimation $L_{opt}\ =\ arg\ \min_{L} f\left(L\right)$. At the same time, the uncertainty of thickness estimation can be evaluated using the curvature of the objective function near L_{opt} : $V_{ar}\left(L_{opt}\right)\approx\sigma_R^2\ H^{-1}$, where $H\approx 2\sum_k w_k\ J_k^2, Jk\ =\ \partial R_{calc}\ /\ \partial L$.

2.2. Model Solution and Results

The established model and algorithm are used to process the infrared spectral data of the silicon carbide wafer (incidence angle of 10° and 15°, respectively) provided by the attachment.

First, the reflectance spectra are preprocessed and interference extreme points (bright and dark) are identified. Figure 1 shows the reflectance-wavenumber curve at an angle of incidence of 10°, where red dots mark the identified bright lines (crests) and green dots mark dark lines (troughs). It can be observed that the reflectance changes sharply in the low-to-midwave range, while in the high-wavelength range (≥1200 cm^{-1}), there is a clear, near-periodic interference fringe, and the extreme point in this region is stable and suitable for thickness calculation.

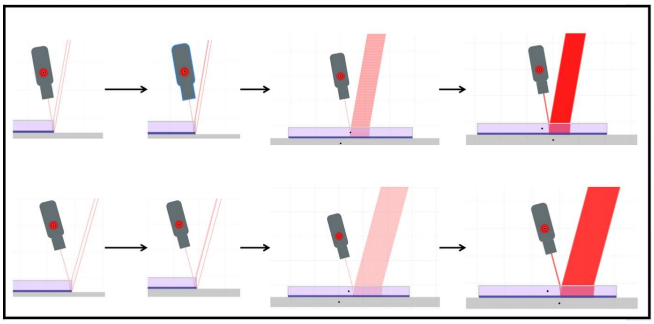

Figure 1 Critical change in light interaction in interference effect (10° above and 15° below, compared to the final light intensity enhancement)

Based on the identified extreme value points, the optimization algorithm is used to calculate the thickness corresponding to each extreme value point, and its average value is calculated. The solution result is shown in the following table 1:

Table 1 Film thickness analysis results

Indicators	Angle of incidence 10°	Angle of incidence 15°
Mean refractive inde	2.1537	2.1926
Number of bright lines	18	18
Number of dark lines	18	18
Average thickness of the surface pattern (μm)	9.9345	9.7911
Average thickness of dark lines (μm)	11.2874	10.9138
Light/dark thickness difference (%)	12.75	10.84
Average thickness (μm)	10.6110	10.3525

The distribution of thickness with wavenumber is shown in Figure 2. In the high wavenumber region, the thickness scatters are closely distributed near the mean, forming a stable platform, indicating that the inversion results are stable and reliable. In the strong dispersion range of ~900-1050 cm^{-1}, due to the rapid change of dielectric constant, the extreme positioning sensitivity and noise amplification are greatly deviated.

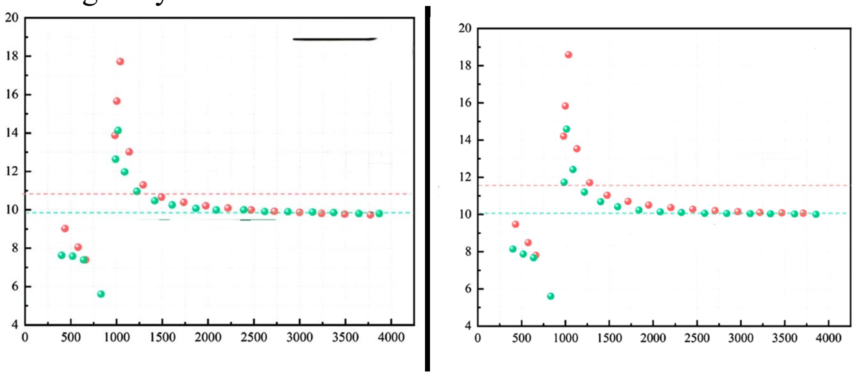

Figure 2 Thickness-wavenumber curve, left (10°), right (15°)

2.3. Results and discussion

Consistency of results: The calculated average thickness of the surface pattern (9.93 μm vs 9.79 μm) and the average thickness of the dark pattern (11.29 μm vs 10.91 μm) were very close at the two angles of incidence of 10° and 15°, with a difference of 1.4% and 3.4%, respectively. This high degree of consistency of cross-angle calculation results strongly proves the reliability and repeatability of the models and algorithms established in this paper.Analysis of the difference in the thickness of light and dark lines: Whether it is 10° or 15° of incidence, the average thickness calculated by the dark pattern is systematically higher than that calculated by the bright pattern, and the thickness difference is between 10% and 13%. This systemic bias can stem from several aspects:

Model simplification: The dual-beam model ignores the multiple reflection effect in the epitaxial layer, and when there are non-negligible multiple reflections, it will affect the phase and amplitude of the interference fringe, resulting in a bias in the inversion based on the position of the extreme point.

Approximation of phase mutation treatment: The treatment of half-wave loss during reflection in the model may have subtle approximations at different interference levels and interfaces.

Extreme point localization error: Although the streaks are clear in the high wavenumber region, the positioning of dark lines (troughs) may be more susceptible to background noise or baseline drift than bright lines (peaks) in some bands.

Algorithm effectiveness: The "simulated annealing + least squares" dual-scale optimization algorithm designed in this paper proves to be effective. The simulated annealing algorithm successfully provides a good initial value for subsequent fine optimization and avoids the local optimal problem. On this basis, the least squares method finds the thickness solution with the highest degree of agreement with the experimental data. The robustness of the algorithm combination can be further verified by sensitivity analysis (e.g., perturbation objective function weights).Measurement accuracy and scope of application: By introducing the Sellmeier equation and the Drude model, the model better handles the dispersion problem of refractive index and improves the physical accuracy of thickness inversion. The stability of the calculated results in the high wavenumber flattening region shows that the proposed method has high measurement accuracy in this region. For the deviation of the strong dispersion interval, it is suggested that we need more complex dispersion models or consider multi-layer structural effects in future work.

3. Conclusion

In this study, focusing on the need for accurate and non-destructive measurement of the thickness of silicon carbide epitaxial layer, the model construction and algorithm optimization based on infrared interferometry are systematically carried out, and the following main conclusions are obtained:

Firstly, a physical model for thickness measurement of silicon carbide epitaxial layer based on the principle of dual-beam interference is successfully established. The model not only clearly describes the basic relationship between interference fringes and epitaxial layer thickness, refractive index and angle of incidence, but more importantly, accurately characterizes the dispersion characteristics of silicon carbide refractive index with wavelength and carrier concentration by introducing the Sellmeier equation and the Drude model, which lays a solid physical foundation for high-precision inversion of thickness. The model derives an analytical expression for calculating the thickness by interference series and extreme point wavelength, with clear principles and clear physical significance.

Secondly, for the inversion problem of physical model, an efficient and robust thickness calculation optimization algorithm is innovatively designed and implemented. The algorithm adopts a bi-scale strategy, combining the global search ability of the simulated annealing algorithm and the local fine optimization ability of the least squares method, which effectively overcomes the local minimum trap in nonlinear optimization and ensures that the thickness estimate close to the global optimal is obtained. The algorithm also enhances the adaptability and robustness of the actual measured data by constructing the error function of the theoretical and experimental reflectances, and considering the average effects of s-polarized and P-polarized light.

Finally, the effectiveness of the proposed model and algorithm is confirmed by processing and verifying the infrared spectral data of actual silicon carbide wafers. At two different angles of incidence (10° and 15°), the calculated epitaxial layer thickness results showed good consistency (about 1.4% difference in surfacegrain thickness), which cross-verified the reliability of the method. Although there is a certain systematic deviation (about 10%-13%) in the calculation results of bright and dark lines, which reveals the limitations of simplifying the two-beam model under specific conditions and points out the necessity of introducing multi-beam interference correction in the future, the models and algorithms provided in this study provide a solution with considerable accuracy and strong stability for the core measurement tasks.

In summary, the silicon carbide epitaxial layer thickness measurement method based on infrared interferometry method and optimization algorithm proposed in this paper has a rigorous theoretical model, robust algorithm design, and reliable experimental results, which provides a valuable reference scheme for the rapid and non-destructive monitoring of silicon carbide epitaxial layer thickness on the semiconductor process line, and has clear practical application potential. Future work will focus on correcting models for multi-beam interference effects to further improve measurement accuracy in complex scenarios such as highly reflective substrates.

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